NIST Standard Reference Database 88

NIST/TRC Ideal Gas Database

Version 1.0

Users' Guide

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The NIST/TRC Ideal Gas Database is a companion software to the book:

"Thermodynamics of Organic Compounds in the Gas State", vol. 1,2. by Michael Frenkel, G. J. Kabo, K. N. Marsh, G. N. Roganov and R. C. Wilhoit: TRC, College Station, TX, 1994 VERSION 1.0

This package contains the NIST/TRC Ideal Gas Database (TRCIDG).

TABLE OF CONTENTS

1. INTRODUCTION

1.1 Database Description

The NIST TRC Ideal Gas database (TRCIDG) provides information on the most important thermodynamic properties (heat capacities, entropies, enthalpies, Gibbs free energies and enthalpies and Gibbs free energies of formation) of organic (and some other) compounds in the ideal gas state. The database contains a total of more than 2000 compounds. The heat capacities are calculated using coefficients of linear or non-linear functions of their temperature dependence. These coefficients were obtained based on the results of statistical mechanical or additive calculations. The other properties (entropies, enthalpies and Gibbs free energies) are determined by integration using a heat capacity function. The enthalpies and Gibbs free energies of formation are calculated based on the properties of the individual compounds and the properties of their elements in the standard states. The calculations can be performed in two different regimes: NON-LINEAR and POLYNOMIAL. The regime POLYNOMIAL uses a linear function to represent temperature dependence of heat capacity. This function is simple and commonly used in engineering applications. However, there may not be a sufficient number of significant digits to insure sufficient accuracy at temperatures higher than 3000 K. When choosing the NON-LINEAR regime, the heat capacities are calculated using the non-linear function of temperature. This function is quite complicated, but it ensures sufficient accuracy over a wide temperature range. The NON-LINEAR regime is the default selection when the user starts running this database.

1.2 Installation

To install the NIST TRC Ideal Gas Database (TRCIDG) on your hard drive, insert the CD-Rom, go to Start/Run and click on the program setup.exe.

***NOTE**: In Windows 98, If no C:\TEMP directory exists go to the your Windows/Explorer and create the directory before beginning the Install process.*

System Requirements: TRCIDG requires hard disk with 110 megabytes of available disk space.

The software may also be run under Microsoft ®Windows 95, 98, 2000 and Windows NT4.0.

Older Systems

On older systems, the config.sys file must contain at least the following configuration:

```
FILES=20
BUFFERS=30
DEVICE=C:\DOS\HIMEM.SYS
```

If the config.sys file does not include the last statement shown above, this program will only use conventional memory instead of using both conventional and extended memory, then it cannot calculate tables for large numbers of compounds at the same time.

NOTE: *that newer systems use the file CONFIG.NT in place of CONFIG.SYS to configure the system for running DOS programs. It is possible to modify these settings for each specific DOS program. Please see CONFIG.NT under INDEX in Windows Help.*

1.3 Running

Note: On Windows 95 systems the default directory offered by TRCIDG for the output files, C:\TEMP, does not exist by default. You must either create this directory prior to execution, or select an existing directory for output. The Ideal Gas database has been tested on Windows 95, 98, 2000 and Windows NT 4.0.

Run the program from the directory C:\Program Files\NIST TRC Databases\Ideal Gas (or wherever you installed it - this is the default location used by the installation program) or from the Start Menu on the Windows Taskbar. Under Programs on the Start Menu, find the tab for NIST TRC Databases and select Ideal Gas. You may find it convenient to create a desktop shortcut to the folder C:\Program Files\NIST TRC Databases. When the default directory box appears hit the enter key to continue.

The program tests for monitor type. Then the user will be asked about the path (directory) in which to put the log file, and whether there is extended memory available. If you want to have the log file located in the current directory, simply type in `.' This path will be used for the log and saved files. When the main program is running, a menu bar appears at the top of the screen, along with a context-sensitive help line at the bottom. To select menu items, move the cursor to the appropriate menu item or type the first character of the menu item and press RETURN. A new menu or screen will appear for the selected item. To exit the current menu or screen, press ESC. Selecting EXIT from the main menu exits the program. Pressing <F1> at any point will bring up a more comprehensive help screen corresponding to the current mode.

TRCIDG also maintains a log file of the calculation results for the compounds selected. *This log file will be overwritten the next time the program is run.* To mark a compound, move the cursor to the compound and press the Enter key or press <F7> to select all the compounds chosen. An asterisk `*' will be displayed telling you that it has been marked. After the calculation is completed, the characters `*' will be replaced by `#'. To reselect these compounds press Enter or press <F7> key twice. If you desire, the file IDG.LOG can be saved to a filename of your choice by invoking the SAVE option (see below).

On the top line of the main menu screen, xxxK means the amount of unused "conventional" memory of your computer. File CAS is a sample file for batch input. File TEMP is a sample file for temperature input.

2. GENERAL INFORMATION.

2.1 Screen Movement

To move the cursor within the list of compound names (Name) or formulas (Formula) obtained from the selection, use the arrows to move the cursor in the appropriate direction. Use the <PageUp> key to move to the previous page or the <PageDown> key to go to the next page. The <Home> key takes you to the first line, the <End> key takes you to last line. To select a compound for a calculation press the <Enter> key. See the help screen (press the <F1> key) for details.

2.2 Screen Search

Function key <F2> searches for any string in the name field. This feature is particularly useful in finding the correct compound when the formula or partial name search gives you a large number of compounds. To select a compound after an <F2> search, the cursor must be on the name, then press <Enter>. Use <F3> to continue the search for the next instance of the string and <F4> to search for the previous match of the string.

2.3 Previous Screen and Previous Menu

The <Esc> key always returns you to the previous screen or menu

2.4 Help Screens

Pressing the <F1> Key at any screen gives help messages corresponding to the highlighted menu box.

2.5 Full Screen vs. Window Usage

You can select between running Ideal Gas in full-screen mode or in its own window. Click the right mouse button on the Ideal Gas icon (or on whatever icon you use to launch the program) to bring up the File menu. Click on Properties to bring up the Properties dialog box. Select the Screen tab. Then select either Full-screen or Window.

Note: that on newer computers the Ideal Gas program runs much faster in full-screen mode.

2.6 Uninstalling TRCIDG

TRCIDG can be uninstalled using "Add/Remove Programs" from the "Control Panel". From the "Start" menu, select "Settings", then select "Control Panel" (or double-click "Control Panel" under "My Computer"). Double-click "Add/Remove Programs". Then scroll down until you find "NIST TRC Ideal Gas". Highlight "NIST TRC Ideal Gas" and then click the "Add/Remove" button.

3. TRCIDG FUNCTIONALITY

3.1 Main Menus

The main menus appears in the upper left hand corner of the screen.

Main Menus
Compound File Exit

To select an option in the main menu either move the highlight using the left or right arrow key to the appropriate option then press <Enter>; or instead, type the first letter corresponding to that option.

Compound: This is the option required for calculating the thermodynamic functions of a specified compound in the ideal gas state.

File: View of all searches and calculations made during the session.

Exit: Exits the program.

3.2 Selection: Compound

The following options are listed in the upper left hand corner of the screen:

Name Formula CASRN Batch

3.2.1 Selection: Name

There are two options for name retrieval:

A) Whole Name Search
B) Partial Name Search

The help screen <F1> describes the options

Several names are included in the database for most compounds. If you do not locate a desired compound with a name search, try the formula search.

3.2.2 Selection: Formula

The format for the formula search is very flexible. See the help screen <F1> for details.

Note: all compounds that match the formula entered will be displayed on the screen.

3.2.3 Selection: CASRN

Retrieves compounds using Chemical Abstract Service Registry Number (CASRN). The number may be entered with hyphens, "-", or with no hyphens but with no check digit.

Example: 1,2-butadiene may be entered as either 590-19-2 or 59019, but NOT 590192.

Only exact matches will be displayed.

The numbers greater than 500000-00-0 have been assigned by TRC, for indexing purposes, to those compounds for which we have no Chemical Abstracts Service Registry Number.

3.2.4 Selection: Batch

This option allows the input of a batch file. You will be asked for the file name and if the file contains CASRN, formulas, or names.

After displaying one or more compounds, move the cursor to the desired compound and press <Enter> to select it. Only one compound can be selected for a vapor pressure calculation.

3.3 Calculations

After the selection of a compound, the following options appear vertically on the right side of the screen.

Non-Linear
Polynomial
Temperature
Choose Units

Non-Linear: This option uses a non-linear function to calculate thermodynamic properties for selected compounds at selected temperatures (see Introduction)

Polynomial: This option uses a linear function to calculate thermodynamic properties for selected compounds at selected temperatures (see Introduction)

Temperature: This selection provides an option to enter required temperatures either from a file generated prior to running TRCIDG (option 0) or from the keyboard (option 1).Option 0 requires the user to specify the full path to the location of the file. Option 1 requires information about the lowest and the highest temperatures, as well as the temperature increment. Additional temperature entries can be added as desired.

Choose Units: If units other than {J/(mol K)} and (K) are desired, they can be selected from the Units screen.

The retrieval software includes the option of converting values from the units used in the database [{J/(mol K)} and (K)] to the desired units to be displayed on the screen. The user selects from the menu provided. The conversion formulas used are:

Temperature (stored as kelvin, K)
Celsius, t/C = T/K - 298.15
Rankine, t/R = 1.8 x T/K
Fahrenheit, t/F = (1.8 x T/K) - 459.67

Thermodynamic functions are stored in {J/(mol K)}. These functions also can be expressed as {J/(g K)}, {cal/(mol K)}, {cal/(g K)}, {BTU/(lb-mol R)}, and {BTU/(lb R)}

The following factors are used for conversion (M-molar mass, N-amount of substance in moles, m-mass, E-energy):
Gram, m/g = N/g-mol x M(g/g-mol)
Pound, m/lb = m/g / 453.59237
Pound per Mole, N/lb-mol = N/g-mol / 453.59237

British Thermal Unit, E/BTU = (E/J) / 1055.056
Calorie, E/cal = (E/J) / 4.184

Note: For a formula or partial name search other compounds can be selected from the previous screen by pressing <Esc>.

3.4 Selection: File

The following list of options appear vertically on the right side of the screen

Review
Save
Print

3.4.1 Selection: Review

This option can be used to review the results of the searches and calculations that have been stored in C:\TEMP\IDG.LOG (by default), in whatever path was chosen by the user at the beginning of execution.

3.4.2 Selection: Save

This option can be used to save the results of the searches and calculations to a user-specified file. By default, results will be saved to the file C:\TEMP\IDG.LOG

IMPORTANT NOTE: IDG.LOG *will be overwritten at the start of the next session or whenever the save command is issued.*

3.4.3 Selection: Print (This feature is deprecated.)

This option can be used to print the results of the searches and calculations to your default printer if this printer is directly connected to your computer. DO NOT use this option if a printer is not *directly* connected to your computer or TRCIDG will hang.

RECOMMENDATION ON PRINTING RESULTS:
In general, it is more effective to first *SAVE* the result to a file, open the file in Word or WordPad, and print the results from there.

CONTACTS

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If you have questions or comments about the database, Standard Reference Data would like to hear from you. Also, if you have any problems with the diskettes or installation, please let us know by contacting:

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